

1-(2,6-Difluorobenzyl)-1H-1,2,3-triazole-4-carboxamide

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|-----------------------------|--|
| Other names: | CGP 33101 E 2080 Inovelon RUF 331 Rufinamide Tox21 112267 |
| Inchi: | InChI=1S/C10H8F2N4O/c11-7-2-1-3-8(12)6(7)4-16-5-9(10(13)17)14-15-16/h1-3,5H,4H2, |
| InchiKey: | POGQSBRIGCQNEG-UHFFFAOYSA-N |
| Formula: | C10H8F2N4O |
| SMILES: | <chem>N=C(O)c1cn(Cc2c(F)cccc2F)nn1</chem> |
| Mol. weight [g/mol]: | 238.19 |
| CAS: | 106308-44-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.45 | | Crippen Method |
| logp | 1.488 | | Crippen Method |
| mcvol | 153.570 | ml/mol | McGowan Method |
| rinpol | 2077.40 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C106308445&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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